



Full wwPDB EM Validation Report ⓘ

Oct 19, 2024 – 08:18 AM EDT

PDB ID : 8DXO
EMDB ID : EMD-27771
Title : Structure of LRRC8C-LRRC8A(IL125) Chimera, Class 2
Authors : Takahashi, H.; Yamada, T.; Denton, J.S.; Strange, K.; Karakas, E.
Deposited on : 2022-08-02
Resolution : 3.60 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

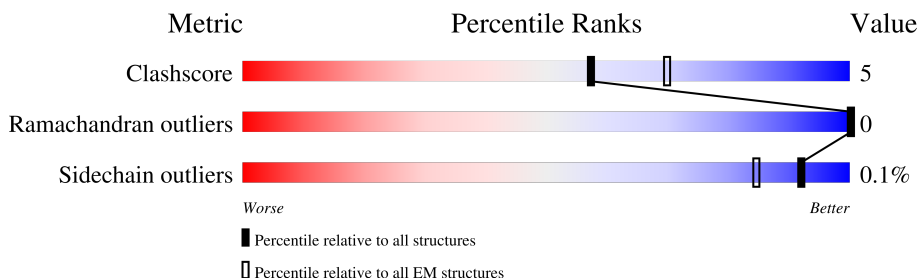
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	825	
1	B	825	
1	C	825	
1	D	825	
1	E	825	
1	F	825	
1	G	825	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 17499 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Volume-regulated anion channel subunit LRRC8C, Volume-regulated anion channel subunit LRRC8A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	298	Total	C	N	O	S	0	0
			2481	1640	391	429	21		
1	B	300	Total	C	N	O	S	0	0
			2501	1653	395	432	21		
1	C	301	Total	C	N	O	S	0	0
			2507	1656	396	434	21		
1	D	300	Total	C	N	O	S	0	0
			2497	1650	393	433	21		
1	E	301	Total	C	N	O	S	0	0
			2507	1656	396	434	21		
1	F	302	Total	C	N	O	S	0	0
			2516	1661	397	437	21		
1	G	299	Total	C	N	O	S	0	0
			2490	1645	392	432	21		

There are 147 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	177G	GLY	-	linker	UNP Q8IWT6
A	?	-	LYS	deletion	UNP Q8TDW0
A	803	GLU	-	expression tag	UNP Q8TDW0
A	804	ASN	-	expression tag	UNP Q8TDW0
A	805	LEU	-	expression tag	UNP Q8TDW0
A	806	TYR	-	expression tag	UNP Q8TDW0
A	807	PHE	-	expression tag	UNP Q8TDW0
A	808	GLN	-	expression tag	UNP Q8TDW0
A	809	GLY	-	expression tag	UNP Q8TDW0
A	810	ALA	-	expression tag	UNP Q8TDW0
A	811	ALA	-	expression tag	UNP Q8TDW0
A	812	ALA	-	expression tag	UNP Q8TDW0
A	813	GLY	-	expression tag	UNP Q8TDW0
A	814	ASP	-	expression tag	UNP Q8TDW0
A	815	TYR	-	expression tag	UNP Q8TDW0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	816	LYS	-	expression tag	UNP Q8TDW0
A	817	ASP	-	expression tag	UNP Q8TDW0
A	818	ASP	-	expression tag	UNP Q8TDW0
A	819	ASP	-	expression tag	UNP Q8TDW0
A	820	ASP	-	expression tag	UNP Q8TDW0
A	821	LYS	-	expression tag	UNP Q8TDW0
B	176H	GLY	-	linker	UNP Q8IWT6
B	?	-	LYS	deletion	UNP Q8TDW0
B	803	GLU	-	expression tag	UNP Q8TDW0
B	804	ASN	-	expression tag	UNP Q8TDW0
B	805	LEU	-	expression tag	UNP Q8TDW0
B	806	TYR	-	expression tag	UNP Q8TDW0
B	807	PHE	-	expression tag	UNP Q8TDW0
B	808	GLN	-	expression tag	UNP Q8TDW0
B	809	GLY	-	expression tag	UNP Q8TDW0
B	810	ALA	-	expression tag	UNP Q8TDW0
B	811	ALA	-	expression tag	UNP Q8TDW0
B	812	ALA	-	expression tag	UNP Q8TDW0
B	813	GLY	-	expression tag	UNP Q8TDW0
B	814	ASP	-	expression tag	UNP Q8TDW0
B	815	TYR	-	expression tag	UNP Q8TDW0
B	816	LYS	-	expression tag	UNP Q8TDW0
B	817	ASP	-	expression tag	UNP Q8TDW0
B	818	ASP	-	expression tag	UNP Q8TDW0
B	819	ASP	-	expression tag	UNP Q8TDW0
B	820	ASP	-	expression tag	UNP Q8TDW0
B	821	LYS	-	expression tag	UNP Q8TDW0
C	177G	GLY	-	linker	UNP Q8IWT6
C	?	-	LYS	deletion	UNP Q8TDW0
C	803	GLU	-	expression tag	UNP Q8TDW0
C	804	ASN	-	expression tag	UNP Q8TDW0
C	805	LEU	-	expression tag	UNP Q8TDW0
C	806	TYR	-	expression tag	UNP Q8TDW0
C	807	PHE	-	expression tag	UNP Q8TDW0
C	808	GLN	-	expression tag	UNP Q8TDW0
C	809	GLY	-	expression tag	UNP Q8TDW0
C	810	ALA	-	expression tag	UNP Q8TDW0
C	811	ALA	-	expression tag	UNP Q8TDW0
C	812	ALA	-	expression tag	UNP Q8TDW0
C	813	GLY	-	expression tag	UNP Q8TDW0
C	814	ASP	-	expression tag	UNP Q8TDW0
C	815	TYR	-	expression tag	UNP Q8TDW0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	816	LYS	-	expression tag	UNP Q8TDW0
C	817	ASP	-	expression tag	UNP Q8TDW0
C	818	ASP	-	expression tag	UNP Q8TDW0
C	819	ASP	-	expression tag	UNP Q8TDW0
C	820	ASP	-	expression tag	UNP Q8TDW0
C	821	LYS	-	expression tag	UNP Q8TDW0
D	178F	GLY	-	linker	UNP Q8IWT6
D	?	-	LYS	deletion	UNP Q8TDW0
D	803	GLU	-	expression tag	UNP Q8TDW0
D	804	ASN	-	expression tag	UNP Q8TDW0
D	805	LEU	-	expression tag	UNP Q8TDW0
D	806	TYR	-	expression tag	UNP Q8TDW0
D	807	PHE	-	expression tag	UNP Q8TDW0
D	808	GLN	-	expression tag	UNP Q8TDW0
D	809	GLY	-	expression tag	UNP Q8TDW0
D	810	ALA	-	expression tag	UNP Q8TDW0
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D	816	LYS	-	expression tag	UNP Q8TDW0
D	817	ASP	-	expression tag	UNP Q8TDW0
D	818	ASP	-	expression tag	UNP Q8TDW0
D	819	ASP	-	expression tag	UNP Q8TDW0
D	820	ASP	-	expression tag	UNP Q8TDW0
D	821	LYS	-	expression tag	UNP Q8TDW0
E	177G	GLY	-	linker	UNP Q8IWT6
E	?	-	LYS	deletion	UNP Q8TDW0
E	803	GLU	-	expression tag	UNP Q8TDW0
E	804	ASN	-	expression tag	UNP Q8TDW0
E	805	LEU	-	expression tag	UNP Q8TDW0
E	806	TYR	-	expression tag	UNP Q8TDW0
E	807	PHE	-	expression tag	UNP Q8TDW0
E	808	GLN	-	expression tag	UNP Q8TDW0
E	809	GLY	-	expression tag	UNP Q8TDW0
E	810	ALA	-	expression tag	UNP Q8TDW0
E	811	ALA	-	expression tag	UNP Q8TDW0
E	812	ALA	-	expression tag	UNP Q8TDW0
E	813	GLY	-	expression tag	UNP Q8TDW0
E	814	ASP	-	expression tag	UNP Q8TDW0
E	815	TYR	-	expression tag	UNP Q8TDW0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	816	LYS	-	expression tag	UNP Q8TDW0
E	817	ASP	-	expression tag	UNP Q8TDW0
E	818	ASP	-	expression tag	UNP Q8TDW0
E	819	ASP	-	expression tag	UNP Q8TDW0
E	820	ASP	-	expression tag	UNP Q8TDW0
E	821	LYS	-	expression tag	UNP Q8TDW0
F	178F	GLY	-	linker	UNP Q8IWT6
F	?	-	LYS	deletion	UNP Q8TDW0
F	803	GLU	-	expression tag	UNP Q8TDW0
F	804	ASN	-	expression tag	UNP Q8TDW0
F	805	LEU	-	expression tag	UNP Q8TDW0
F	806	TYR	-	expression tag	UNP Q8TDW0
F	807	PHE	-	expression tag	UNP Q8TDW0
F	808	GLN	-	expression tag	UNP Q8TDW0
F	809	GLY	-	expression tag	UNP Q8TDW0
F	810	ALA	-	expression tag	UNP Q8TDW0
F	811	ALA	-	expression tag	UNP Q8TDW0
F	812	ALA	-	expression tag	UNP Q8TDW0
F	813	GLY	-	expression tag	UNP Q8TDW0
F	814	ASP	-	expression tag	UNP Q8TDW0
F	815	TYR	-	expression tag	UNP Q8TDW0
F	816	LYS	-	expression tag	UNP Q8TDW0
F	817	ASP	-	expression tag	UNP Q8TDW0
F	818	ASP	-	expression tag	UNP Q8TDW0
F	819	ASP	-	expression tag	UNP Q8TDW0
F	820	ASP	-	expression tag	UNP Q8TDW0
F	821	LYS	-	expression tag	UNP Q8TDW0
G	178F	GLY	-	linker	UNP Q8IWT6
G	?	-	LYS	deletion	UNP Q8TDW0
G	803	GLU	-	expression tag	UNP Q8TDW0
G	804	ASN	-	expression tag	UNP Q8TDW0
G	805	LEU	-	expression tag	UNP Q8TDW0
G	806	TYR	-	expression tag	UNP Q8TDW0
G	807	PHE	-	expression tag	UNP Q8TDW0
G	808	GLN	-	expression tag	UNP Q8TDW0
G	809	GLY	-	expression tag	UNP Q8TDW0
G	810	ALA	-	expression tag	UNP Q8TDW0
G	811	ALA	-	expression tag	UNP Q8TDW0
G	812	ALA	-	expression tag	UNP Q8TDW0
G	813	GLY	-	expression tag	UNP Q8TDW0
G	814	ASP	-	expression tag	UNP Q8TDW0
G	815	TYR	-	expression tag	UNP Q8TDW0

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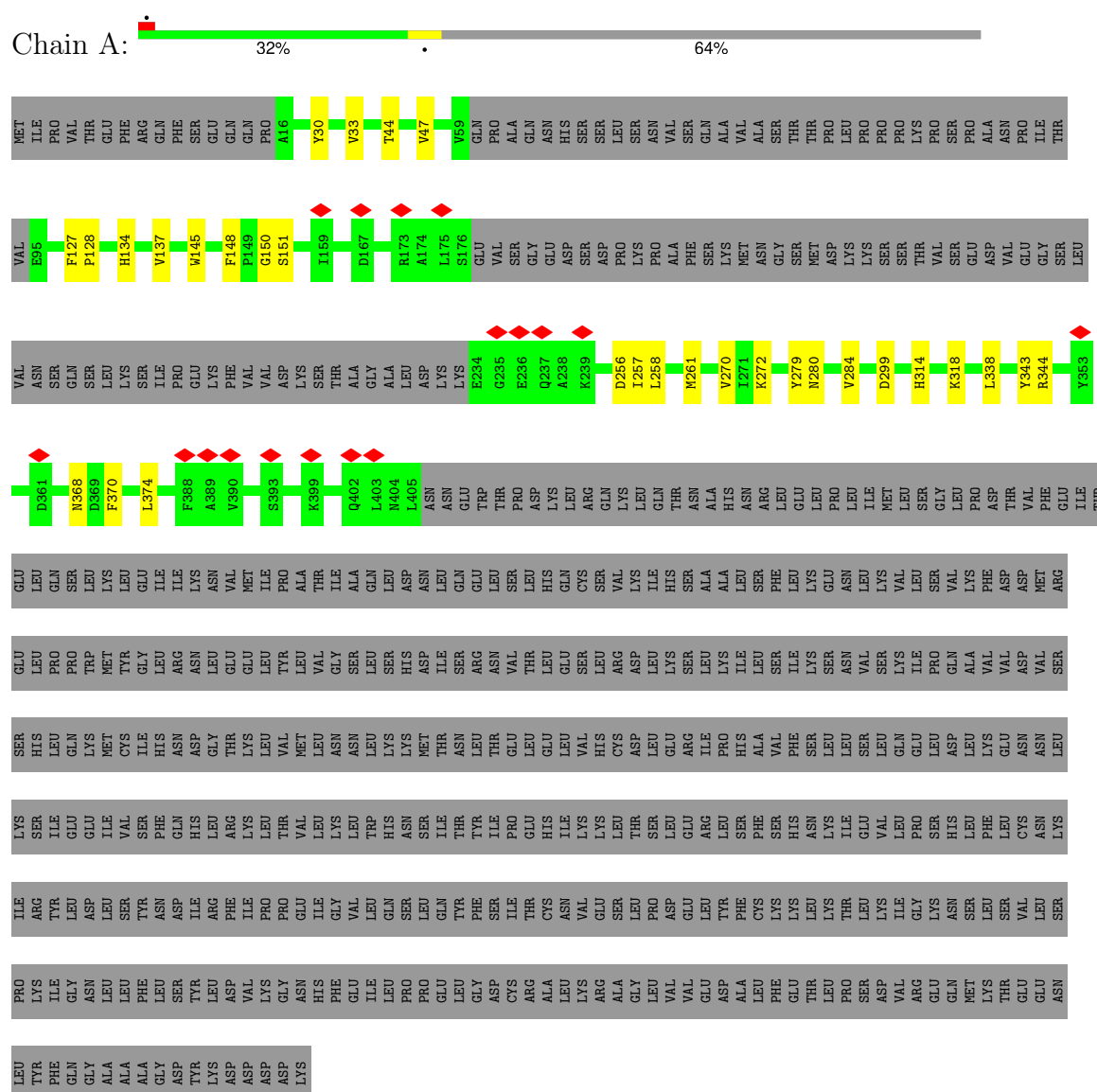
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Chain	Residue	Modelled	Actual	Comment	Reference
G	816	LYS	-	expression tag	UNP Q8TDW0
G	817	ASP	-	expression tag	UNP Q8TDW0
G	818	ASP	-	expression tag	UNP Q8TDW0
G	819	ASP	-	expression tag	UNP Q8TDW0
G	820	ASP	-	expression tag	UNP Q8TDW0
G	821	LYS	-	expression tag	UNP Q8TDW0

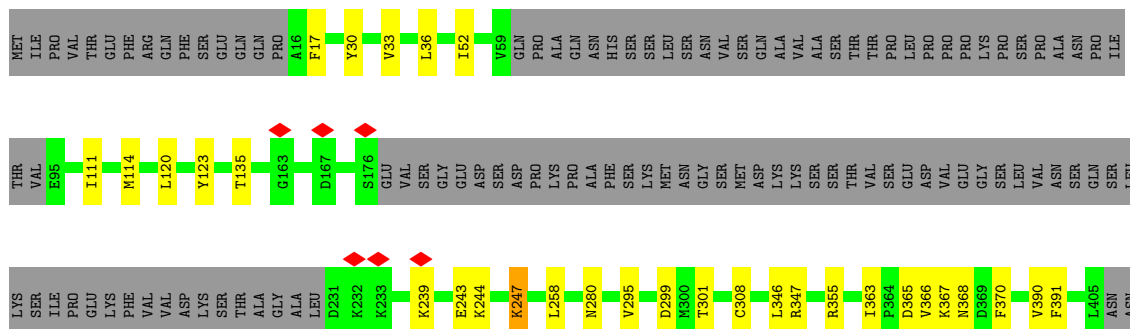
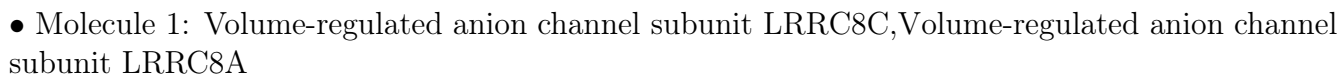
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Volume-regulated anion channel subunit LRRC8C, Volume-regulated anion channel subunit LRRC8A

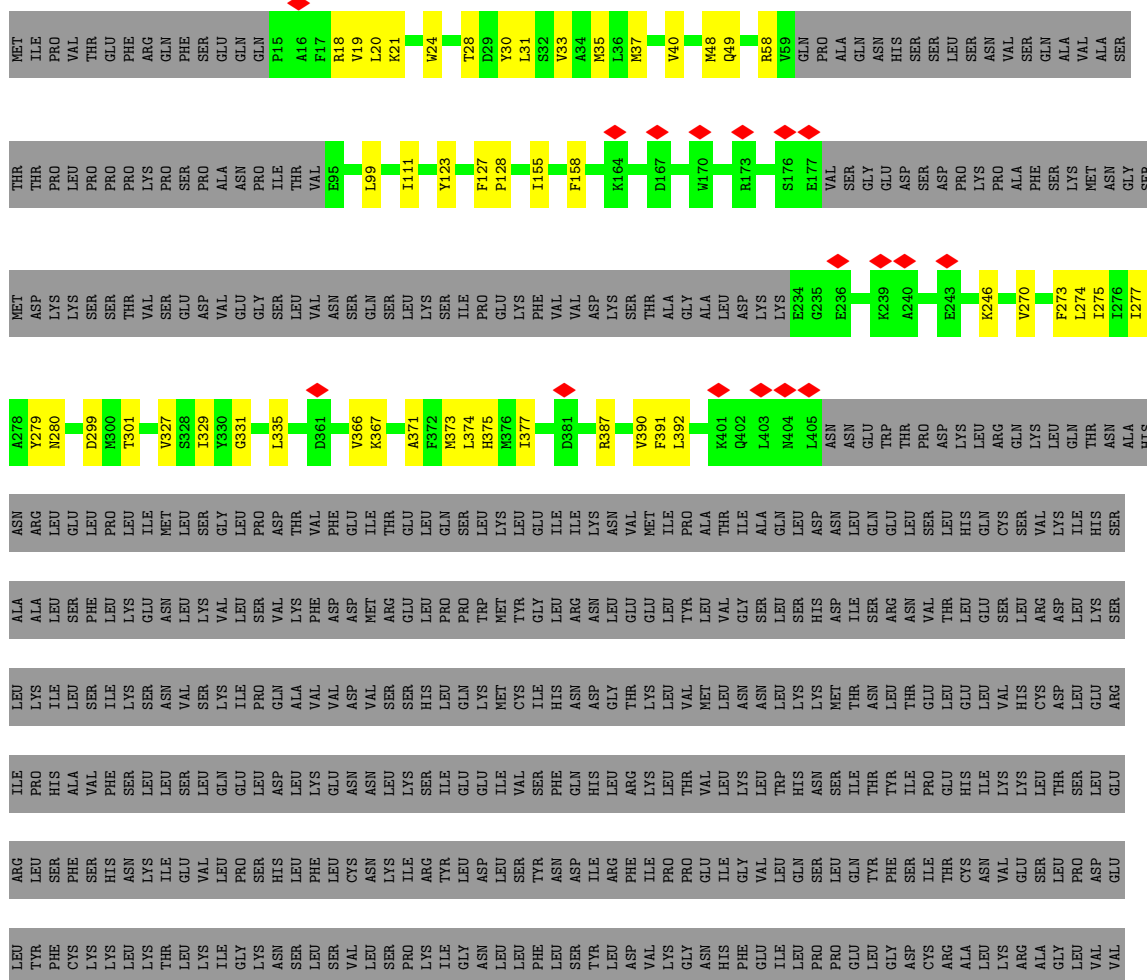


- Chain B: 32% 64%



PRO	GLU	LEU	SER	MET	ASP	ASN	GLU
LEU	GLN	ILE	THR	THR	ILE	LEU	TRP
LEU	TYR	THR	ASN	ASN	SER	GLN	THR
GLY	PHE	TYR	LEU	LEU	ARG	GLU	PRO
ASP	SER	ILE	THR	THR	ASN	LEU	LYS
CYS	ILE	PRO	GLU	GLU	VAL	SER	LEU
ARG	THR	GLU	GLU	GLU	THR	LEU	LEU
ALA	CYS	HIS	GLU	GLU	LEU	HIS	ARG
LEU	ASN	ILE	LEU	GLN	SER	GLN	LYS
LEU	VAL	ILE	VAL	VAL	SER	CYS	LYS
ARG	GLU	LEU	HIS	HIS	LEU	SER	LEU
ALA	SER	LEU	CYS	CYS	ARG	VAL	GLN
GLY	LEU	THR	ASP	ASP	ASP	LYS	THR
LEU	PRO	SER	LEU	LEU	LEU	ILE	ASN
VAL	ASP	LEU	GLU	GLU	LYS	HIS	ALA
VAL	GLU	GLU	ARG	ILE	LEU	ALA	ASN
GLU	TYR	SER	LEU	PRO	LYS	ALA	ARG
ASP	PHE	SER	SER	HIS	ILE	LEU	LEU
ALA	CYS	PHE	PHE	ALA	ILE	LEU	LEU
LEU	LYS	SER	VAL	VAL	SER	SER	GLU
PHE	LYS	SER	VAL	VAL	LEU	PHE	LEU
GLU	LYS	HIS	PHE	PHE	ILE	LEU	PRO
THR	LEU	ASN	SER	SER	LYS	LYS	LEU
LEU	LYS	LYS	LEU	LEU	SER	GLU	ILE
PRO	THR	ILE	LEU	LEU	ASN	ASN	MET
SER	LEU	GLU	SER	SER	VAL	LEU	LEU
ASP	LYS	VAL	LEU	LYS	VAL	LYS	SER
VAL	ILE	ILE	GLN	GLN	LYS	VAL	GLY
ARG	GLY	PRO	GLU	GLU	ILE	LEU	LEU
GLU	LYS	SER	LEU	LEU	PRO	SER	PRO
GLN	ASN	HIS	ASP	ASP	GLN	VAL	ASP
LEU	LEU	LEU	ASN	ASN	ASP	ASP	GLU
ASN	SER	LYS	ASN	ASN	VAL	MET	ILE
LEU	SER	ILE	LEU	SER	VAL	ARG	THR
LEU	PRO	ILE	LYS	SER	SER	GLU	GLU
TYR	GLY	ARG	SER	HIS	LEU	LEU	LEU
PHE	ILE	TYR	ILE	ILE	LEU	PRO	GLN
GLN	GLY	GLN	GLU	GLU	GLN	PRO	SER
GLY	ASN	ASP	ASP	GLU	LYS	TRP	LEU
ALA	LEU	LEU	ILE	ILE	MET	MET	LYS
ALA	LEU	SER	VAL	VAL	CYS	TYR	LEU
ALA	PHE	TYR	SER	SER	ILE	GLY	GLU
GLY	LEU	ASN	PHE	PHE	HIS	LEU	ILE
ASP	SER	ASP	GLN	GLN	ASN	ARG	ILE
TYR	TYR	ILE	HIS	HIS	ASP	ASN	LYS
LYS	ASP	ARG	LEU	ARG	GLY	LEU	ASN
ASP	ASP	PHE	ASN	ASN	THR	GLU	VAL
ASP	VAL	ILE	ILE	LYS	LYS	GLU	THR
ASP	VAL	ILE	ILE	LYS	LYS	GLU	ALA
ASP	GLY	PRO	THR	VAL	VAL	TYR	PRO
LYS	ASN	GLU	VAL	VAL	MET	LEU	ALA
		ILE	LYS	LEU	ASN	VAL	THR
		GLY	LYS	LYS	ASN	GLY	ILE
		VAL	LEU	LYS	ASN	SER	ILE
		LEU	TRP	LEU	LEU	LEU	GLN
		GLN	HIS	ASN	LYS	SER	LEU
		SER	ASN	THR	LYS	THR	ASP

- Molecule 1: Volume-regulated anion channel subunit LRRC8C, Volume-regulated anion channel subunit LRRC8A



- Molecule 1: Volume-regulated anion channel subunit LRRC8C, Volume-regulated anion channel subunit LRRC8A

[illegible]

- Molecule 1: Volume-regulated anion channel subunit LRRC8C, Volume-regulated anion channel subunit LRRC8A

ASN	GLN	LEU	LYS	PHE	VAL	ASP	THR	ALA	GLY	LEU	D231	K239	A240	L241	F242	E243	F248	V252	E253	E254	C255	D256	Y262	Q265	L268	K272	I276	Y279	C308	M312	R347	I360	V366													
ASN	GLN	LEU	LYS	PHE	VAL	ASP	THR	ALA	GLY	LEU	D231	K239	A240	L241	F242	E243	F248	V252	E253	E254	C255	D256	Y262	Q265	L268	K272	I276	Y279	C308	M312	R347	I360	V366													
LYS	PRO	PRO	ALA	ASN	PRO	THR	E95	L105	E117	L120	H134	C141	D167	E177	VAL	GLY	GLY	ASP	ASP	LYS	PRO	ALA	PHE	LYS	ASN	GLY	MET	ASP	LYS	SER	THR	VAL	GLY	VAL												
MET	ILE	VAL	THR	GLU	PHE	ARG	PHE	SER	GLU	GLN	PRO	A16	Y30	V33	A34	M35	L36	M37	I38	G39	V40	F41	L45	Q46	I52	V59	GLN	PRO	ALA	GLN	ASN	HTS	SER	LEU	SER	ASN	VAL	SER	GLN	ALA	VAL	VAL	THR	PRO	PRO	PRO

SER TYR LEU ASP VAL LYS GLY ASN HIS PHE GLU ILE LEU PRO PRO GLU LEU GLY ASP CYS ARG ALA LEU LYS ARG ALA GLY VAL VAL GLU ASP ALA LEU PHE GLU THR LEU PRO SER ASP VAL ARG GLU GLN MET LYS THR GLU GLU ASN LEU TYR PHE GLN GLY ALA ALA GLY

ASP TYR LYS ASP ASP ASP LYS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	132722	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	54	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.622	Depositor
Minimum map value	-0.969	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.12	Depositor
Map size (\AA)	396.0, 396.0, 396.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.1, 1.1, 1.1	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.26	0/2548	0.45	0/3441
1	B	0.26	0/2568	0.47	0/3466
1	C	0.26	0/2574	0.46	0/3474
1	D	0.25	0/2565	0.45	0/3464
1	E	0.26	0/2574	0.45	0/3474
1	F	0.26	0/2583	0.45	0/3486
1	G	0.26	0/2557	0.46	0/3453
All	All	0.26	0/17969	0.45	0/24258

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2481	0	2471	20	0
1	B	2501	0	2496	25	0
1	C	2507	0	2501	22	0
1	D	2497	0	2485	30	0
1	E	2507	0	2501	11	0
1	F	2516	0	2507	27	0
1	G	2490	0	2477	27	0
All	All	17499	0	17438	160	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (160) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:134:HIS:NE2	1:F:279:TYR:OH	2.20	0.75
1:C:355:ARG:NH2	1:C:365:ASP:OD1	2.21	0.73
1:E:355:ARG:NH2	1:E:363:ILE:O	2.25	0.69
1:G:134:HIS:NE2	1:G:279:TYR:OH	2.26	0.69
1:A:343:TYR:OH	1:A:344:ARG:NH2	2.25	0.68
1:B:162:LEU:HD13	1:B:388:PHE:CZ	2.28	0.68
1:A:314:HIS:ND1	1:B:117:GLU:OE1	2.27	0.68
1:D:19:VAL:HG23	1:D:20:LEU:HD12	1.77	0.67
1:B:351:PHE:O	1:B:355:ARG:NE	2.28	0.66
1:A:270:VAL:HG21	1:A:338:LEU:HD12	1.78	0.65
1:A:134:HIS:NE2	1:A:279:TYR:OH	2.27	0.65
1:B:259:TYR:OH	1:B:346:LEU:HD13	1.98	0.64
1:E:351:PHE:O	1:E:355:ARG:NH1	2.31	0.64
1:B:331:GLY:O	1:B:335:LEU:HD23	2.01	0.61
1:A:257:ILE:HG23	1:A:258:LEU:CD2	2.31	0.61
1:G:162:LEU:HD23	1:G:388:PHE:CZ	2.36	0.61
1:G:166:PHE:O	1:G:387:ARG:NH2	2.34	0.61
1:B:388:PHE:O	1:B:392:LEU:HD23	2.02	0.60
1:C:239:LYS:O	1:C:243:GLU:OE1	2.20	0.59
1:G:270:VAL:HG21	1:G:338:LEU:CD1	2.32	0.58
1:D:24:TRP:O	1:D:28:THR:HG23	2.03	0.58
1:F:254:GLU:N	1:F:254:GLU:OE1	2.36	0.58
1:A:257:ILE:HG23	1:A:258:LEU:HD22	1.85	0.58
1:C:347:ARG:O	1:C:368:ASN:N	2.33	0.58
1:A:256:ASP:OD1	1:A:368:ASN:ND2	2.37	0.58
1:E:141:CYS:SG	1:E:268:LEU:HD23	2.45	0.57
1:G:123:TYR:OH	1:G:280:ASN:OD1	2.23	0.56
1:D:331:GLY:O	1:D:335:LEU:HD23	2.06	0.56
1:B:358:THR:HG23	1:B:360:ILE:H	1.70	0.56
1:F:105:LEU:HD23	1:F:105:LEU:O	2.06	0.56
1:D:387:ARG:O	1:D:390:VAL:HG22	2.06	0.55
1:G:294:ASN:OD1	1:G:305:ASN:ND2	2.37	0.55
1:G:351:PHE:O	1:G:355:ARG:NE	2.39	0.55
1:D:123:TYR:OH	1:D:280:ASN:OD1	2.20	0.55
1:B:31:LEU:HD11	1:B:329:ILE:HG22	1.89	0.55
1:G:47:VAL:HG23	1:G:47:VAL:O	2.08	0.54
1:G:390:VAL:HG23	1:G:391:PHE:HD1	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:396:SER:O	1:G:400:LEU:HD23	2.08	0.54
1:B:128:PRO:O	1:B:132:LEU:HD23	2.08	0.53
1:F:394:GLU:N	1:F:394:GLU:OE1	2.41	0.53
1:E:314:HIS:ND1	1:F:117:GLU:OE1	2.38	0.53
1:D:31:LEU:O	1:D:35:MET:HG3	2.09	0.52
1:C:30:TYR:O	1:C:33:VAL:HG12	2.10	0.52
1:A:280:ASN:O	1:A:284:VAL:HG23	2.10	0.52
1:C:390:VAL:HG13	1:C:391:PHE:CD2	2.45	0.51
1:B:349:TYR:CD2	1:B:374:LEU:HD23	2.46	0.51
1:B:162:LEU:HD13	1:B:388:PHE:CE2	2.46	0.51
1:A:134:HIS:HE2	1:A:279:TYR:HH	1.52	0.51
1:C:111:ILE:HD11	1:C:301:THR:HG21	1.92	0.51
1:F:241:LEU:HD23	1:F:391:PHE:HE2	1.76	0.50
1:B:355:ARG:HA	1:B:358:THR:HG22	1.94	0.50
1:C:36:LEU:HB2	1:C:135:THR:HG21	1.94	0.50
1:G:162:LEU:HD23	1:G:388:PHE:HZ	1.75	0.50
1:E:52:ILE:HD11	1:E:308:CYS:HB3	1.94	0.50
1:E:132:LEU:O	1:E:136:LEU:HD23	2.11	0.50
1:A:370:PHE:CE2	1:A:374:LEU:HD11	2.46	0.50
1:F:256:ASP:OD2	1:F:347:ARG:NH2	2.45	0.49
1:A:44:THR:O	1:A:47:VAL:HG12	2.12	0.49
1:D:18:ARG:O	1:D:21:LYS:NZ	2.27	0.49
1:D:270:VAL:O	1:D:274:LEU:HD23	2.12	0.49
1:G:287:VAL:O	1:G:287:VAL:HG13	2.12	0.49
1:C:366:VAL:HG12	1:C:367:LYS:N	2.28	0.49
1:B:164:LYS:O	1:B:164:LYS:HD2	2.13	0.49
1:D:277:ILE:HD11	1:D:327:VAL:HG23	1.94	0.49
1:B:391:PHE:O	1:B:392:LEU:HD22	2.14	0.48
1:G:270:VAL:HG21	1:G:338:LEU:HD11	1.93	0.48
1:D:371:ALA:O	1:D:375:HIS:ND1	2.46	0.48
1:D:391:PHE:C	1:D:392:LEU:HD12	2.33	0.48
1:B:128:PRO:HA	1:B:131:VAL:HG12	1.95	0.48
1:B:355:ARG:NH1	1:B:365:ASP:OD1	2.46	0.48
1:C:366:VAL:HG11	1:C:370:PHE:HD2	1.78	0.48
1:G:134:HIS:HA	1:G:137:VAL:HG12	1.94	0.48
1:G:52:ILE:HD11	1:G:308:CYS:HB3	1.97	0.47
1:G:127:PHE:HB3	1:G:128:PRO:HD3	1.97	0.47
1:C:258:LEU:HD23	1:C:258:LEU:O	2.15	0.47
1:D:31:LEU:HD11	1:D:329:ILE:HG22	1.96	0.47
1:F:52:ILE:HD11	1:F:308:CYS:HB3	1.96	0.47
1:C:52:ILE:HD11	1:C:308:CYS:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:248:PHE:CZ	1:F:252:VAL:HG21	2.49	0.47
1:F:35:MET:O	1:F:38:ILE:HG22	2.14	0.47
1:F:52:ILE:HD11	1:F:308:CYS:CB	2.44	0.47
1:B:360:ILE:O	1:B:362:ASP:N	2.45	0.47
1:G:296:ASP:O	1:G:296:ASP:OD1	2.33	0.47
1:G:243:GLU:HA	1:G:243:GLU:OE2	2.15	0.47
1:A:148:PHE:HD2	1:A:151:SER:HG	1.62	0.47
1:D:158:PHE:HZ	1:D:377:ILE:HD12	1.80	0.47
1:B:272:LYS:O	1:B:276:ILE:HG12	2.15	0.46
1:A:134:HIS:HA	1:A:137:VAL:HG12	1.97	0.46
1:D:58:ARG:HH21	1:D:99:LEU:HD13	1.79	0.46
1:B:378:ASP:OD1	1:B:379:GLN:N	2.49	0.46
1:F:95:GLU:N	1:F:95:GLU:OE1	2.48	0.46
1:E:374:LEU:HA	1:E:377:ILE:HG22	1.97	0.46
1:D:299:ASP:N	1:D:299:ASP:OD1	2.49	0.46
1:C:299:ASP:OD1	1:C:299:ASP:N	2.49	0.46
1:D:390:VAL:HG23	1:D:391:PHE:HD1	1.80	0.46
1:F:30:TYR:O	1:F:33:VAL:HG12	2.15	0.45
1:D:20:LEU:HD22	1:D:155:ILE:HD11	1.98	0.45
1:D:30:TYR:O	1:D:33:VAL:HG12	2.16	0.45
1:G:164:LYS:HB3	1:G:241:LEU:HD11	1.99	0.45
1:A:137:VAL:HG21	1:A:272:LYS:HE3	1.99	0.45
1:F:34:ALA:O	1:F:37:MET:HG2	2.17	0.45
1:C:366:VAL:HG12	1:C:367:LYS:H	1.80	0.45
1:G:162:LEU:HD23	1:G:388:PHE:CE2	2.52	0.45
1:F:52:ILE:HD12	1:F:120:LEU:HD13	1.98	0.44
1:F:37:MET:HA	1:F:40:VAL:HG12	1.99	0.44
1:B:137:VAL:HG11	1:B:272:LYS:HE2	1.99	0.44
1:B:162:LEU:HD13	1:B:388:PHE:HZ	1.80	0.44
1:D:275:ILE:O	1:D:279:TYR:CD1	2.71	0.44
1:G:128:PRO:O	1:G:132:LEU:HD13	2.18	0.44
1:A:30:TYR:O	1:A:33:VAL:HG12	2.18	0.44
1:D:366:VAL:HG12	1:D:367:LYS:N	2.33	0.44
1:C:17:PHE:O	1:C:17:PHE:CD2	2.71	0.44
1:C:52:ILE:HD11	1:C:308:CYS:CB	2.47	0.44
1:F:167:ASP:OD1	1:F:167:ASP:N	2.51	0.44
1:F:41:PHE:CZ	1:F:45:LEU:HD11	2.53	0.44
1:C:52:ILE:HD12	1:C:120:LEU:HD13	1.99	0.43
1:A:127:PHE:HB3	1:A:128:PRO:HD3	1.99	0.43
1:C:52:ILE:HD12	1:C:120:LEU:CD1	2.48	0.43
1:C:123:TYR:OH	1:C:280:ASN:OD1	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:270:VAL:HG21	1:G:338:LEU:HD12	1.99	0.43
1:D:111:ILE:HD11	1:D:301:THR:HG21	2.01	0.43
1:E:299:ASP:OD1	1:E:299:ASP:N	2.50	0.43
1:F:52:ILE:HD12	1:F:120:LEU:CD1	2.49	0.43
1:F:272:LYS:O	1:F:276:ILE:HG12	2.19	0.43
1:G:18:ARG:NH1	1:G:380:TYR:OH	2.51	0.43
1:G:374:LEU:HA	1:G:377:ILE:HG22	2.01	0.43
1:F:46:GLN:HA	1:F:312:MET:SD	2.59	0.42
1:D:48:MET:SD	1:D:49:GLN:HG3	2.59	0.42
1:E:171:THR:HG22	1:E:390:VAL:HG11	2.00	0.42
1:F:239:LYS:O	1:F:243:GLU:OE1	2.38	0.42
1:B:349:TYR:CG	1:B:374:LEU:HD23	2.53	0.42
1:F:360:ILE:HG13	1:F:360:ILE:O	2.20	0.42
1:A:314:HIS:O	1:A:318:LYS:HG2	2.20	0.42
1:C:346:LEU:HD12	1:C:346:LEU:O	2.19	0.42
1:D:273:PHE:CE1	1:D:327:VAL:O	2.73	0.42
1:E:240:ALA:O	1:E:243:GLU:HG3	2.20	0.42
1:A:148:PHE:O	1:A:150:GLY:N	2.53	0.41
1:A:299:ASP:OD1	1:A:299:ASP:N	2.53	0.41
1:C:355:ARG:NH2	1:C:363:ILE:O	2.53	0.41
1:D:20:LEU:HD21	1:D:373:MET:CE	2.50	0.41
1:E:36:LEU:HB2	1:E:135:THR:HG21	2.01	0.41
1:C:114:MET:SD	1:C:295:VAL:HG11	2.61	0.41
1:F:262:TYR:O	1:F:265:GLN:HG2	2.21	0.41
1:G:137:VAL:HG11	1:G:272:LYS:HE2	2.01	0.41
1:B:156:GLU:HA	1:B:159:ILE:HG22	2.02	0.41
1:D:391:PHE:O	1:D:392:LEU:HD12	2.20	0.41
1:D:246:LYS:HD3	1:D:246:LYS:N	2.36	0.41
1:D:374:LEU:HA	1:D:377:ILE:HG22	2.02	0.41
1:F:369:ASP:O	1:F:373:MET:HG2	2.20	0.41
1:B:134:HIS:NE2	1:B:279:TYR:OH	2.53	0.41
1:F:366:VAL:HG12	1:F:367:LYS:N	2.36	0.41
1:D:21:LYS:HG3	1:D:21:LYS:O	2.22	0.40
1:G:378:ASP:OD1	1:G:379:GLN:N	2.54	0.40
1:C:244:LYS:O	1:C:247:LYS:HG3	2.20	0.40
1:A:145:TRP:CD1	1:A:261:MET:SD	3.14	0.40
1:D:37:MET:O	1:D:40:VAL:HG12	2.21	0.40
1:F:141:CYS:SG	1:F:268:LEU:HD22	2.62	0.40
1:B:374:LEU:HA	1:B:377:ILE:HG22	2.03	0.40
1:D:127:PHE:HB3	1:D:128:PRO:HD3	2.04	0.40
1:G:155:ILE:O	1:G:159:ILE:HG12	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	292/825 (35%)	277 (95%)	15 (5%)	0	100	100
1	B	294/825 (36%)	272 (92%)	22 (8%)	0	100	100
1	C	295/825 (36%)	276 (94%)	19 (6%)	0	100	100
1	D	294/825 (36%)	274 (93%)	20 (7%)	0	100	100
1	E	295/825 (36%)	281 (95%)	14 (5%)	0	100	100
1	F	296/825 (36%)	272 (92%)	24 (8%)	0	100	100
1	G	293/825 (36%)	273 (93%)	20 (7%)	0	100	100
All	All	2059/5775 (36%)	1925 (94%)	134 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	275/766 (36%)	275 (100%)	0	100	100
1	B	277/766 (36%)	276 (100%)	1 (0%)	89	95
1	C	278/766 (36%)	277 (100%)	1 (0%)	89	95
1	D	277/766 (36%)	277 (100%)	0	100	100
1	E	278/766 (36%)	278 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	279/766 (36%)	279 (100%)	0	100	100
1	G	276/766 (36%)	276 (100%)	0	100	100
All	All	1940/5362 (36%)	1938 (100%)	2 (0%)	92	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	344	ARG
1	C	247	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	265	GLN
1	A	310	HIS
1	B	46	GLN
1	B	237	GLN
1	B	294	ASN
1	C	251	HIS
1	D	157	HIS
1	E	112	ASN
1	E	280	ASN
1	G	298	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

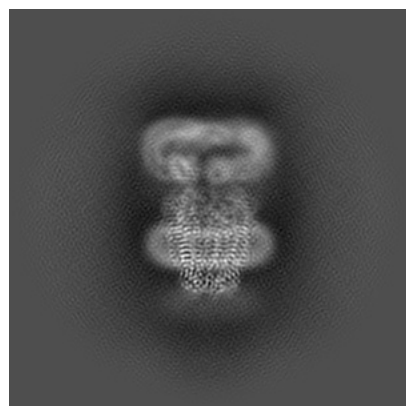
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27771. These allow visual inspection of the internal detail of the map and identification of artifacts.

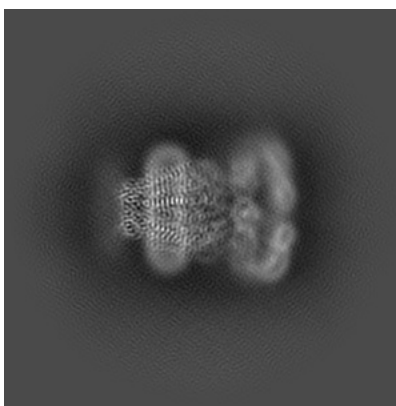
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

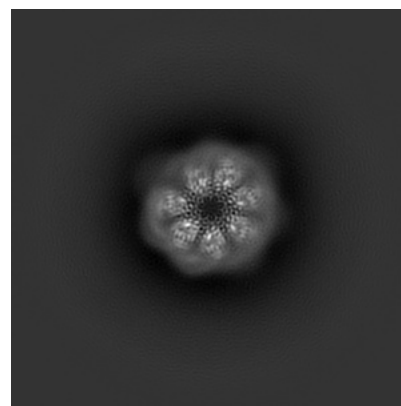
6.1.1 Primary map



X

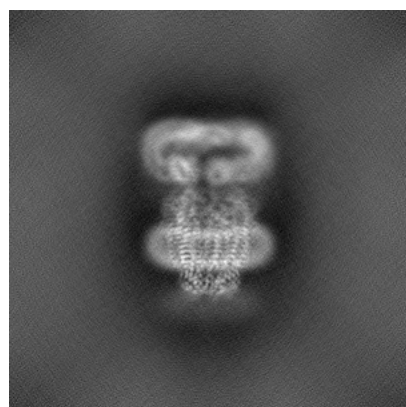


Y

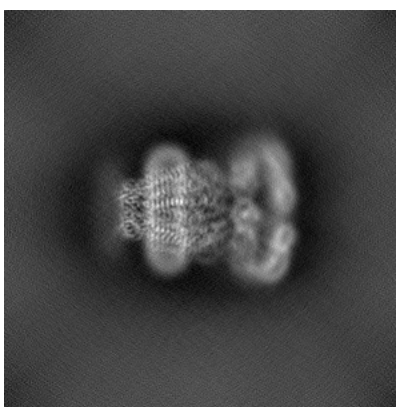


Z

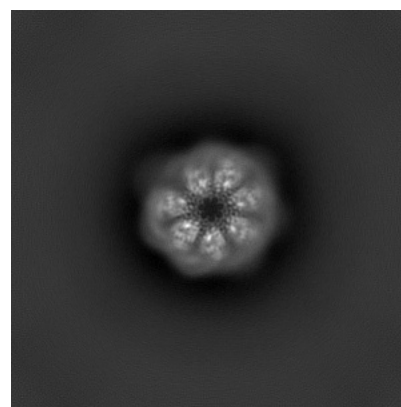
6.1.2 Raw map



X



Y

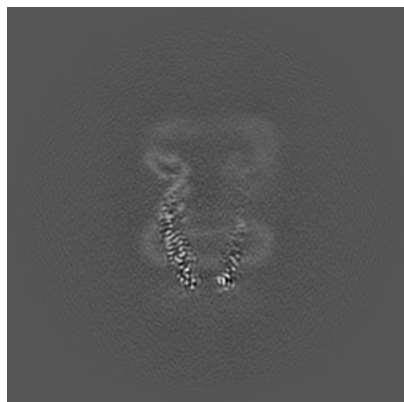


Z

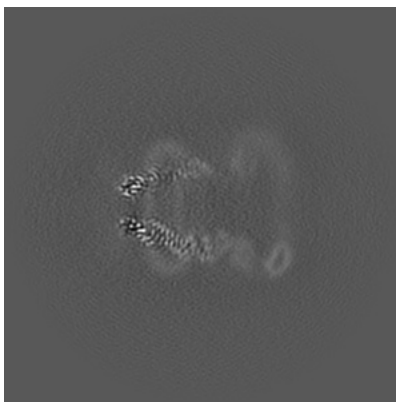
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

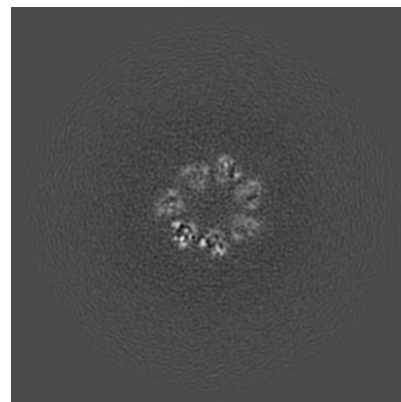
6.2.1 Primary map



X Index: 180

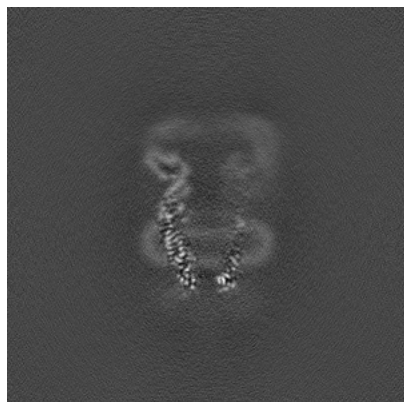


Y Index: 180

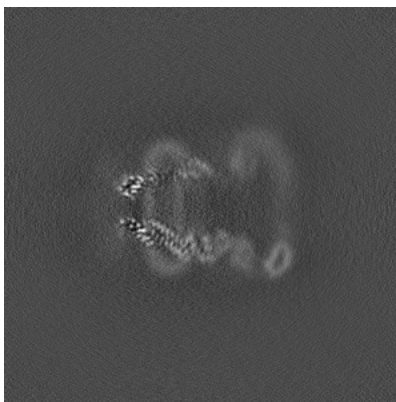


Z Index: 180

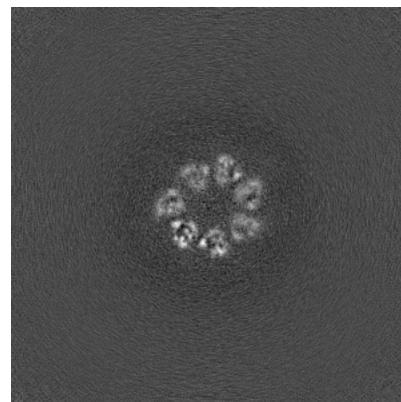
6.2.2 Raw map



X Index: 180



Y Index: 180

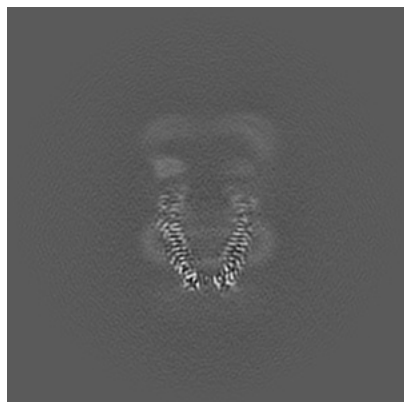


Z Index: 180

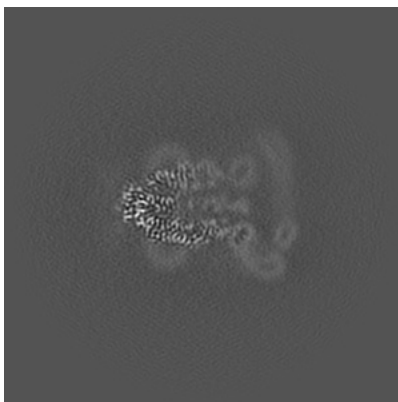
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

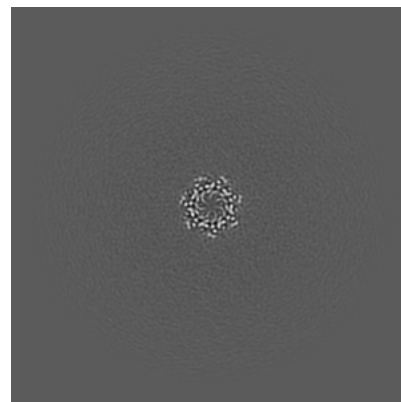
6.3.1 Primary map



X Index: 187

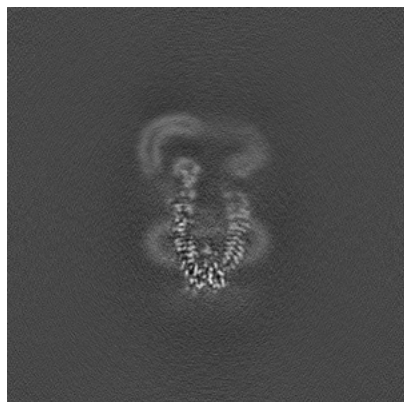


Y Index: 159

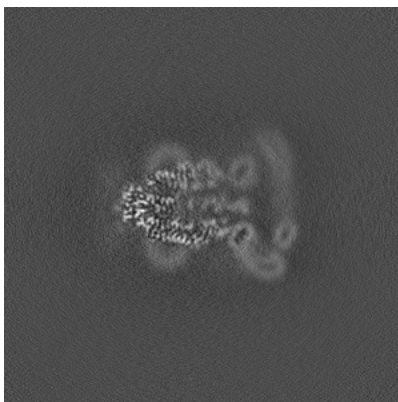


Z Index: 117

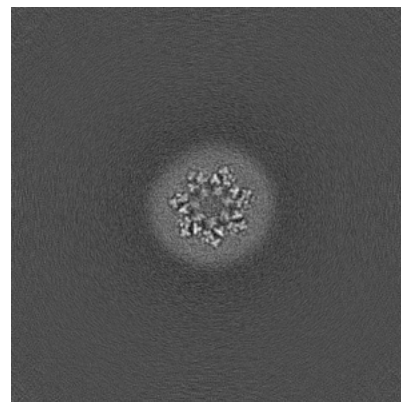
6.3.2 Raw map



X Index: 161



Y Index: 159



Z Index: 133

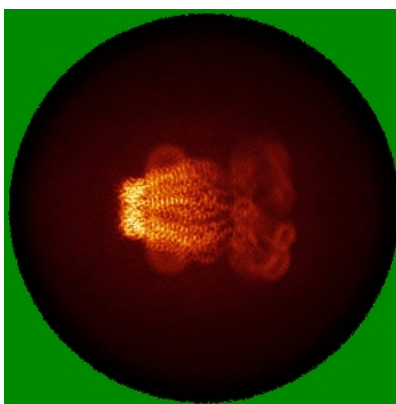
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

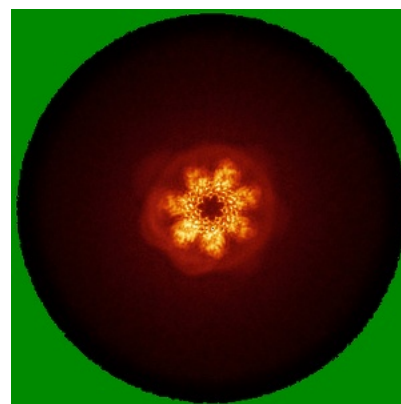
6.4.1 Primary map



X

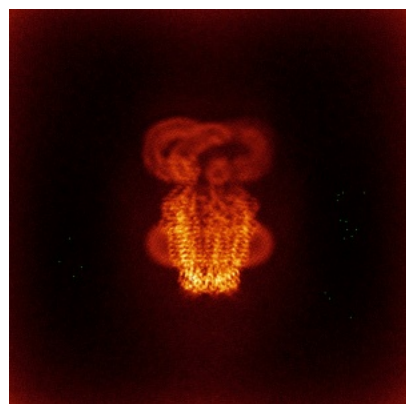


Y

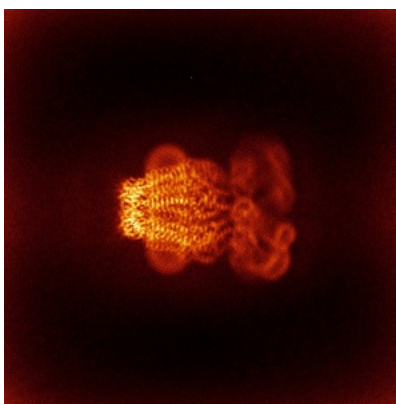


Z

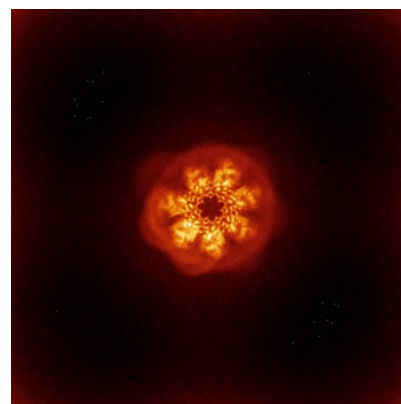
6.4.2 Raw map



X



Y

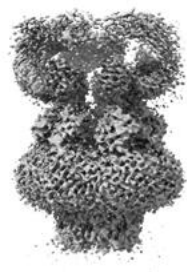


Z

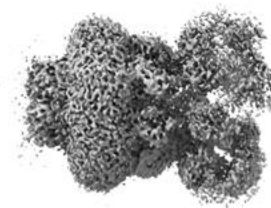
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

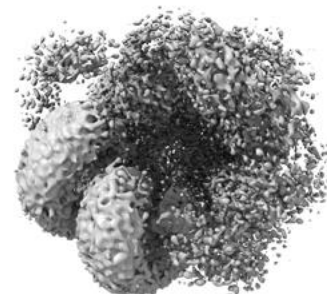
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

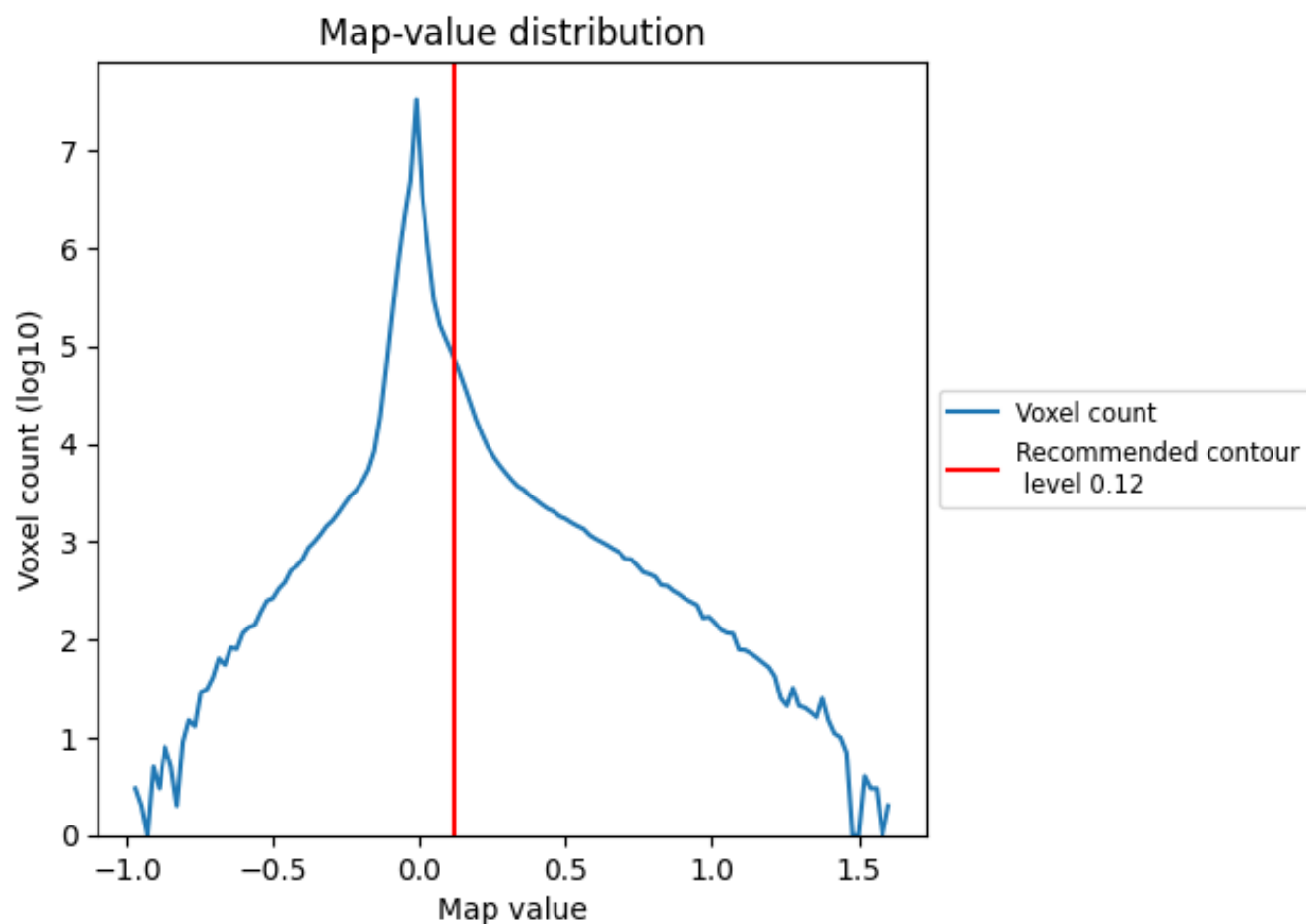
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

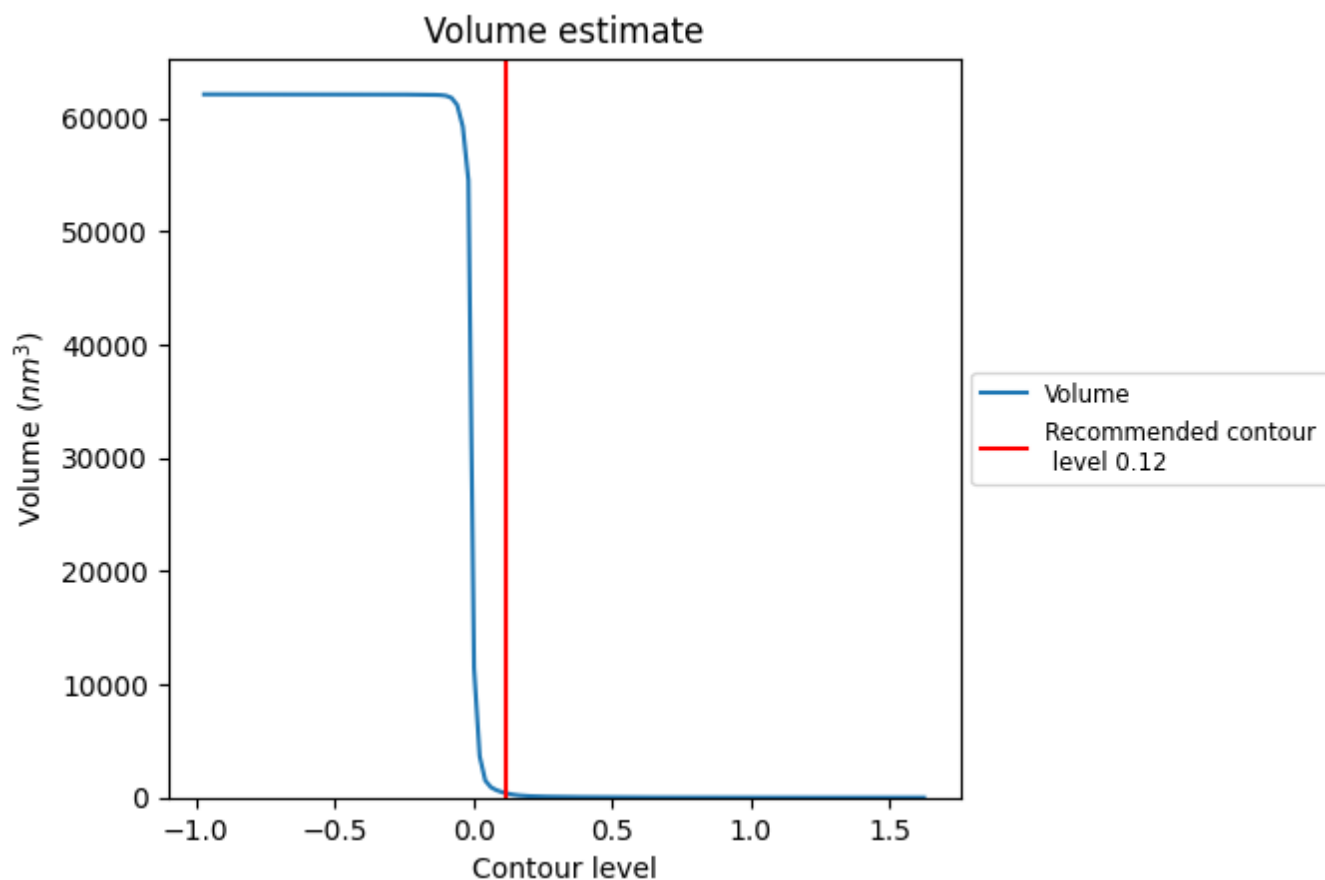
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

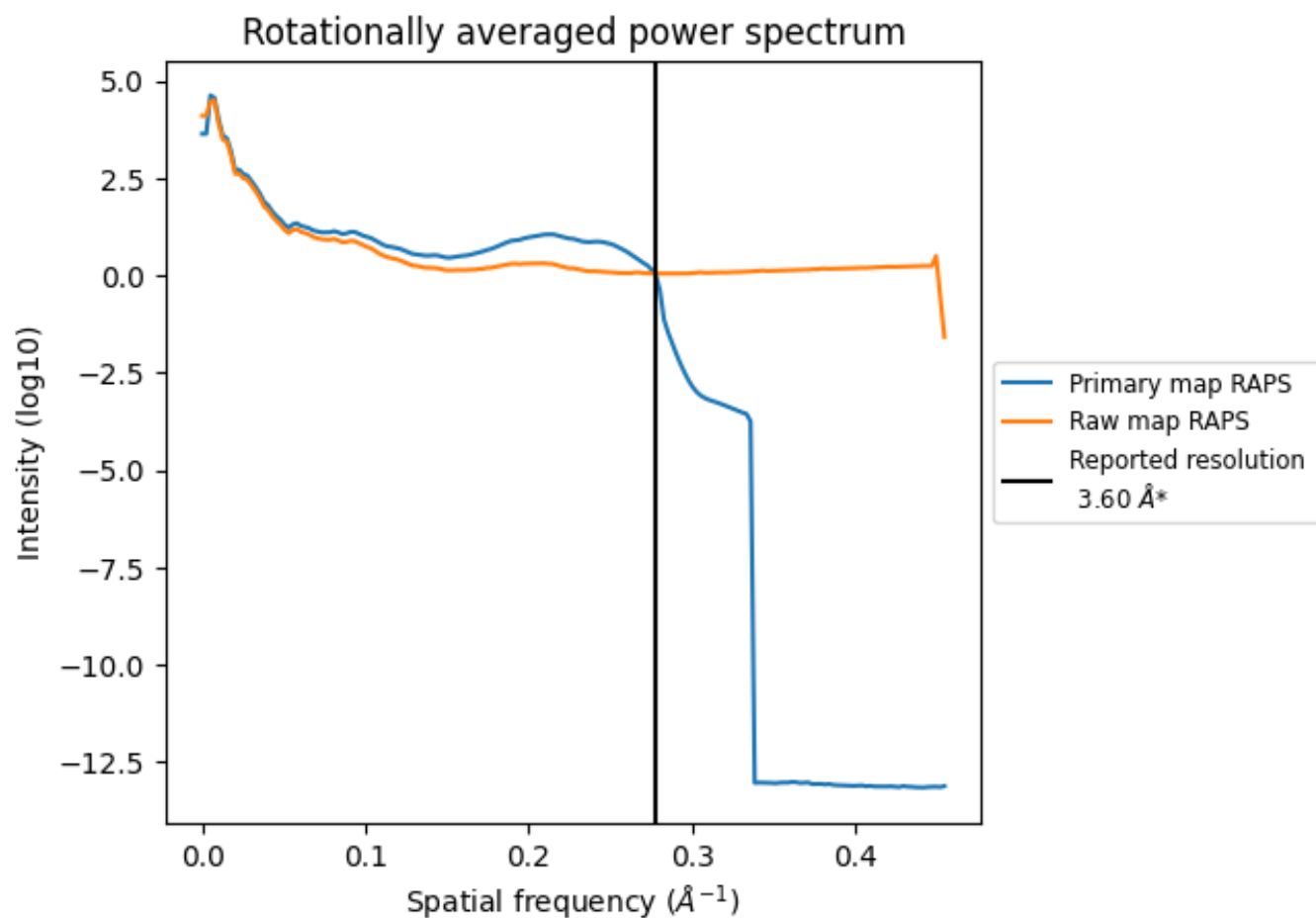
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 371 nm^3 ; this corresponds to an approximate mass of 335 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

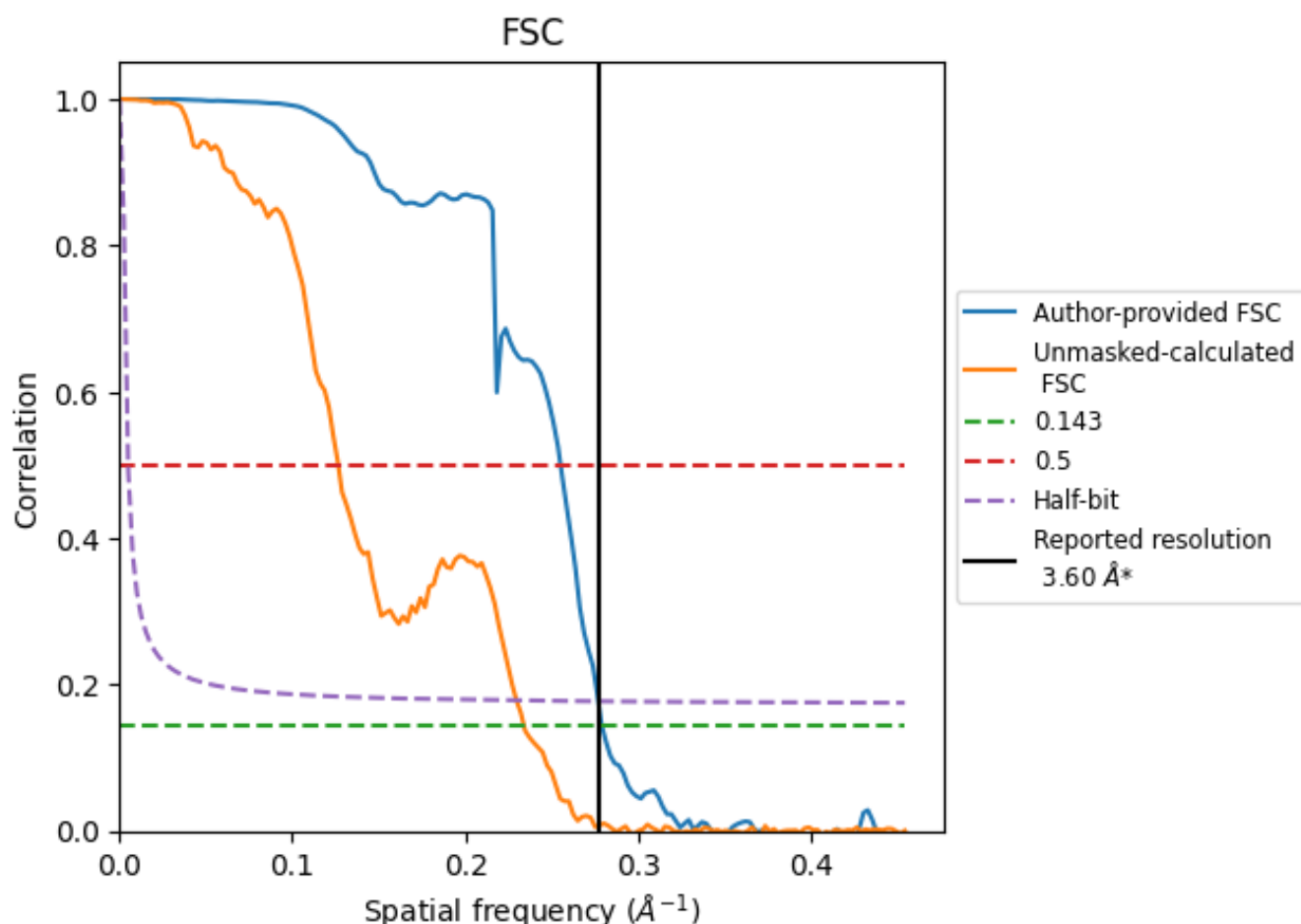


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.278 \AA^{-1}

8.2 Resolution estimates [i](#)

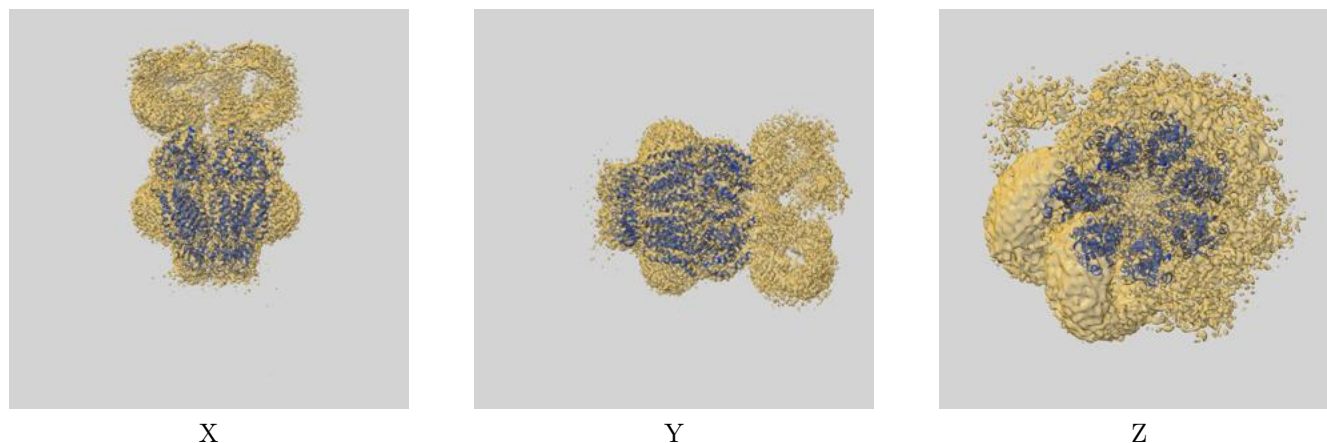
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.58	3.92	3.61
Unmasked-calculated*	4.27	7.90	4.35

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.27 differs from the reported value 3.6 by more than 10 %

9 Map-model fit [i](#)

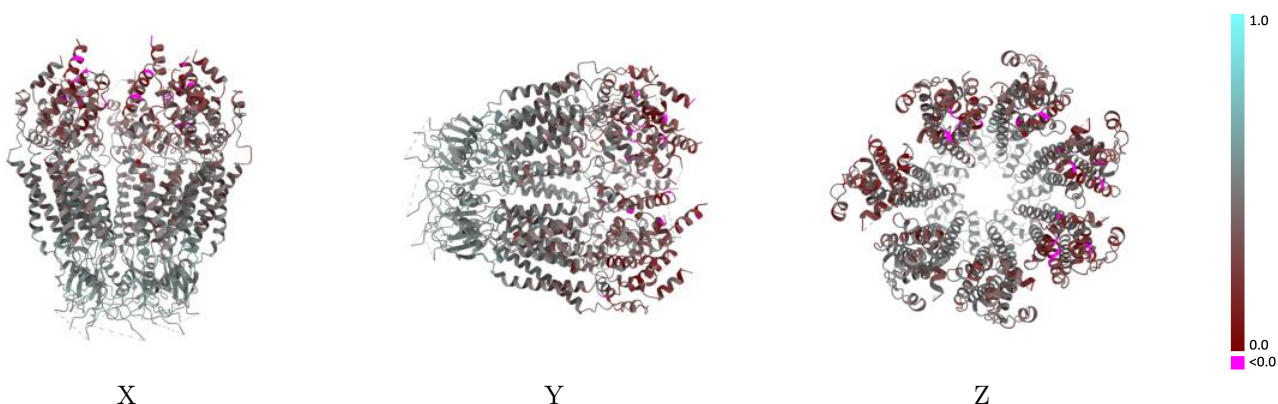
This section contains information regarding the fit between EMDB map EMD-27771 and PDB model 8DXO. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



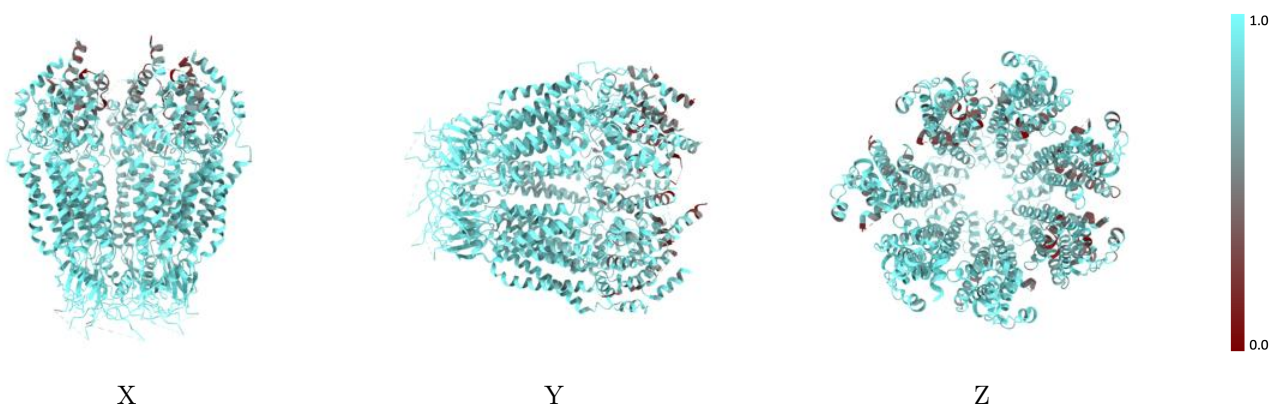
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



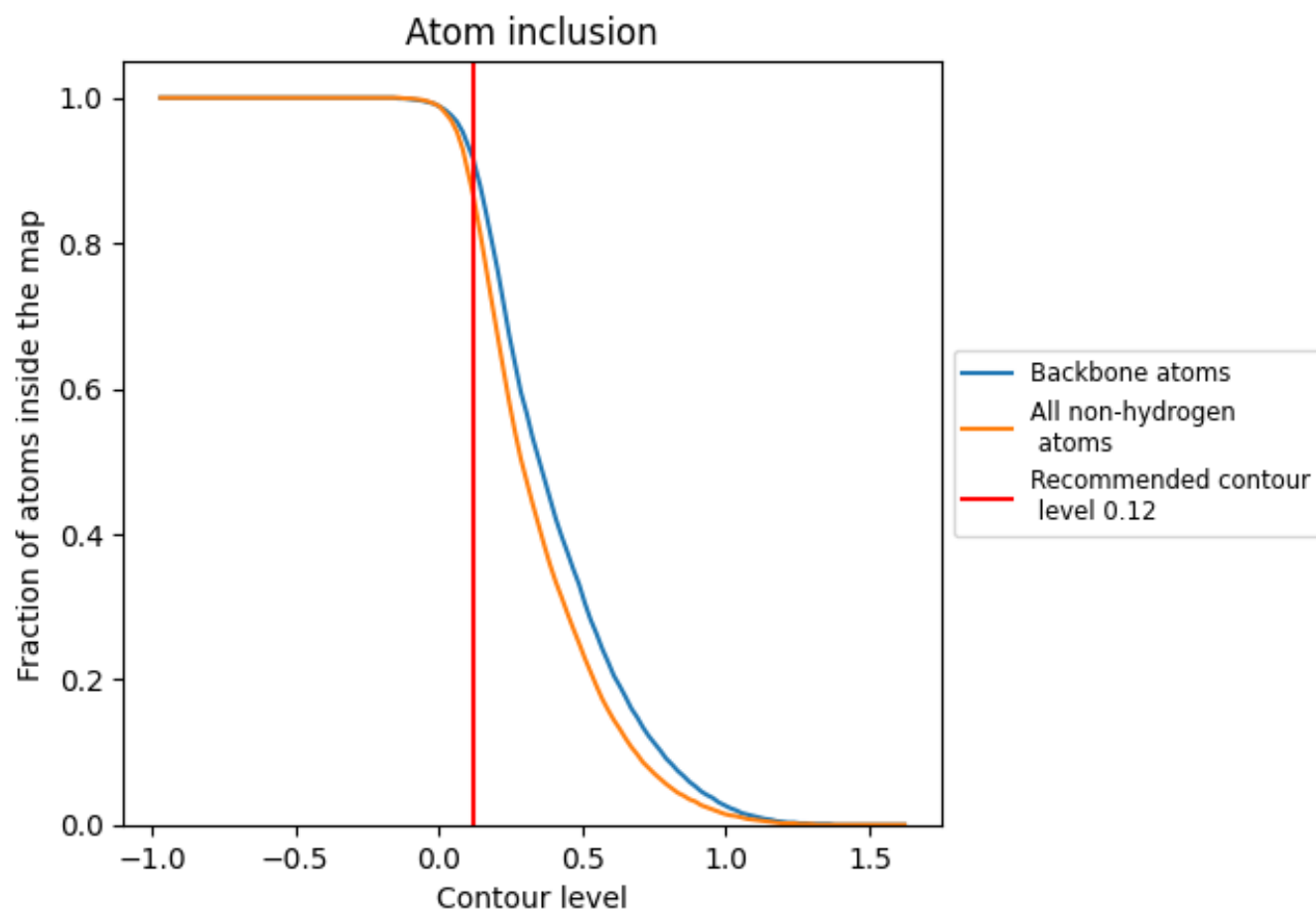
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8660	<div><div></div></div> 0.4220
A	<div><div></div></div> 0.8320	<div><div></div></div> 0.3910
B	<div><div></div></div> 0.8490	<div><div></div></div> 0.4100
C	<div><div></div></div> 0.8780	<div><div></div></div> 0.4330
D	<div><div></div></div> 0.8220	<div><div></div></div> 0.3950
E	<div><div></div></div> 0.8590	<div><div></div></div> 0.4020
F	<div><div></div></div> 0.9180	<div><div></div></div> 0.4660
G	<div><div></div></div> 0.9010	<div><div></div></div> 0.4590

1.0

0.0

<0.0